

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 4.68e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.91e-01

Confidence level: 4.99e-01

Nearest Neighbors from the Training Set

Image not found

phenyl heptopyranoside

Measured: 2.79e-02

Predicted: 1.26e-01

Image not found

Gibberellic acid

Measured: 1.44e-02

Predicted: 5.69e-03